

User Manual: Running the script of BrainPepPass

Welcome to the user manual for BrainPepPass in Google Colab! This is a basic guide for users who wish to perform the prediction of peptide penetration into the blood-brain barrier. Follow each of the steps below to effectively utilize this tool.

Step 1: Uploading of peptides.

When accessing the application link, the user will be directed to the initial screen of BrainPepPass hosted on Google Colab (Figure 1). The first step to execute the script is to upload your peptides in .mol format. If the screen with the session files data is not appearing, click on the Files icon (highlighted in Figure 2). After clicking the icon, a left-hand screen will appear, showing all the uploaded and generated files during program execution (Figure 3).

To upload the .mol files, the user can open the workspace where the files are located and drag them to the session files area. Another way to upload the files is by clicking on the **upload to session storage** button (highlighted in Figure 3), which will direct the user to their local computer's workspace to choose the files and perform the upload.

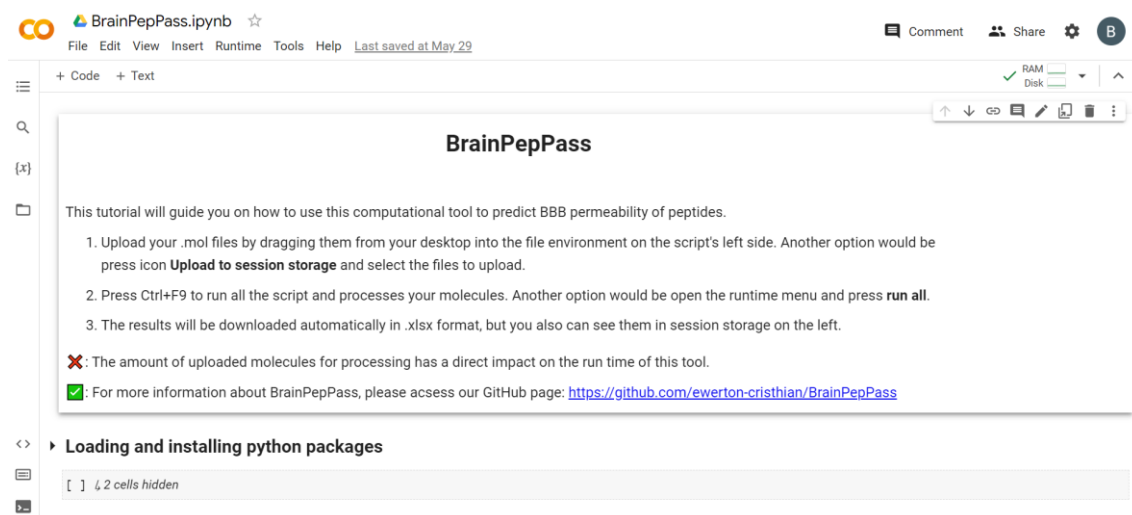


Figure 1: The initial screen of the BrainPepPass application hosted in Google Colab.

After selecting the peptides in .mol format, these files will be displayed on the session storage screen (Fig 4). If your files do not appear on this screen after uploading, click the Refresh button (highlighted in Fig 4).

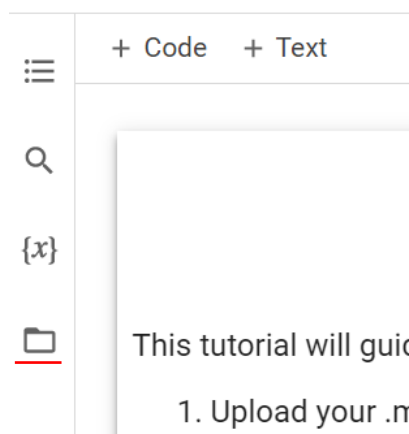


Figure 2: Files icon to open the session storage.

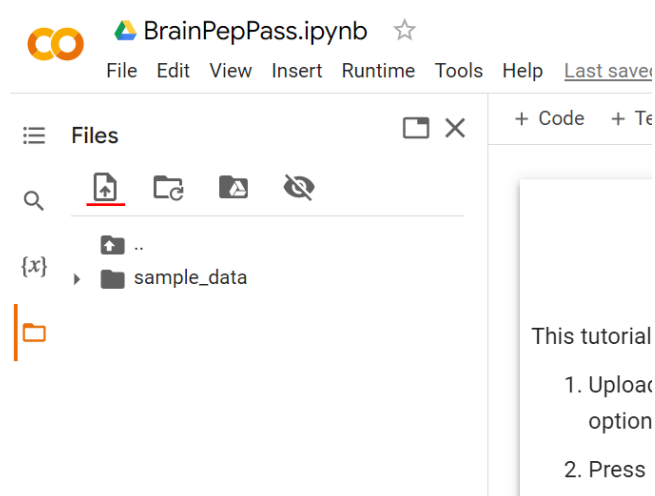


Figure 3: Upload to session storage button.

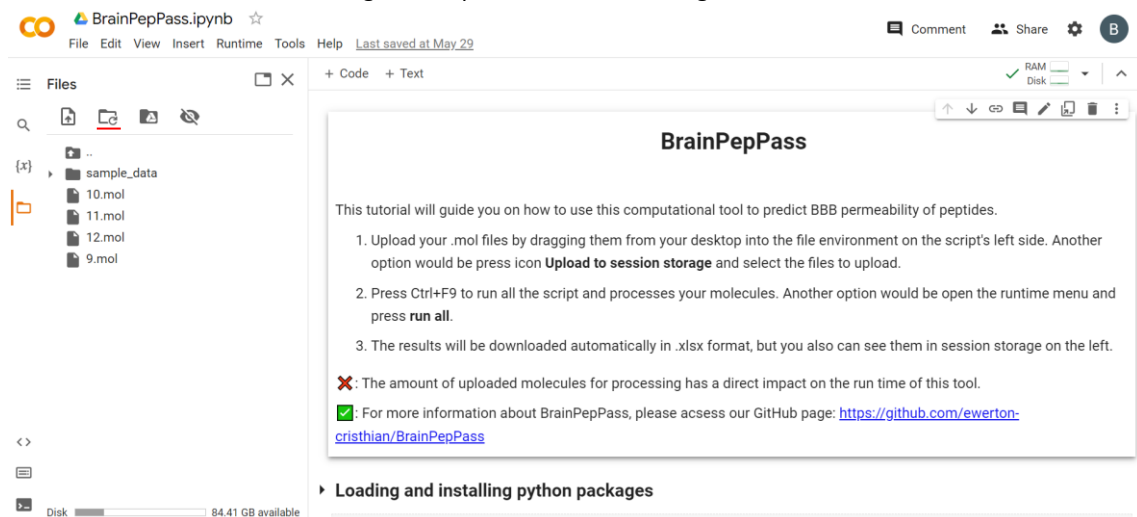


Figure 4: Uploaded .mol files and Refresh button.

Step 2: Script execution.

To run the BrainPepPass system after uploading the peptides, the user can press the Ctrl+F9 buttons, which will execute the system in its entirety. Another way to run the system is by clicking on the Runtime option in the taskbar and selecting the Run all option (Figure 5).

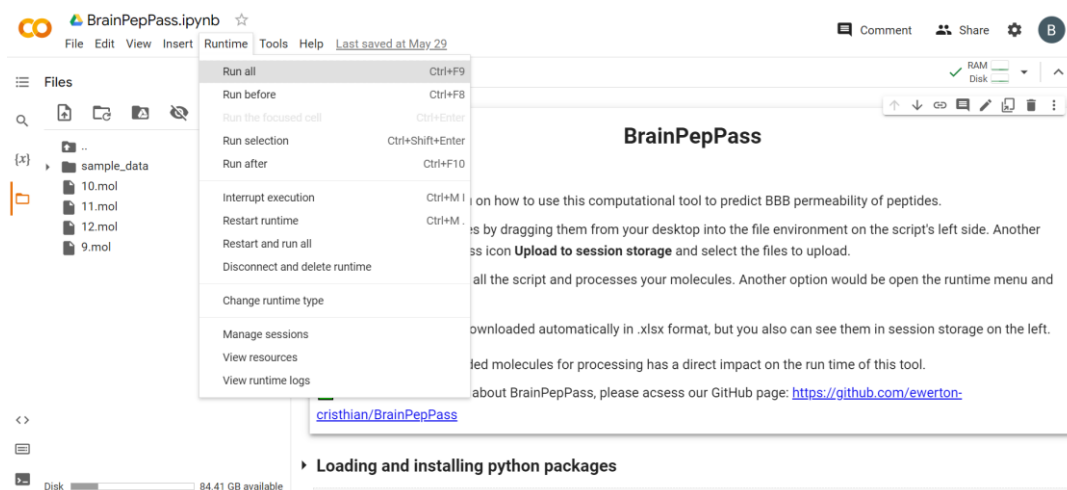


Figure 5: Run all option to run BrainPepPass system.

When running the system for the first time, the process may take a few extra seconds to complete as some necessary files and packages will be downloaded for the first time.

Once the execution is finished, a file named **BrainPepPass_results.xlsx** containing the prediction results will be automatically downloaded by your web browser. This file will also be available in the session storage for you to download (Figure 6). The BrainPepPass can be run again with new data, just follow all the steps in this manual.

It is important to point out that the uploaded files and the results will be lost as soon as the user leaves the Google Colab page with the application.

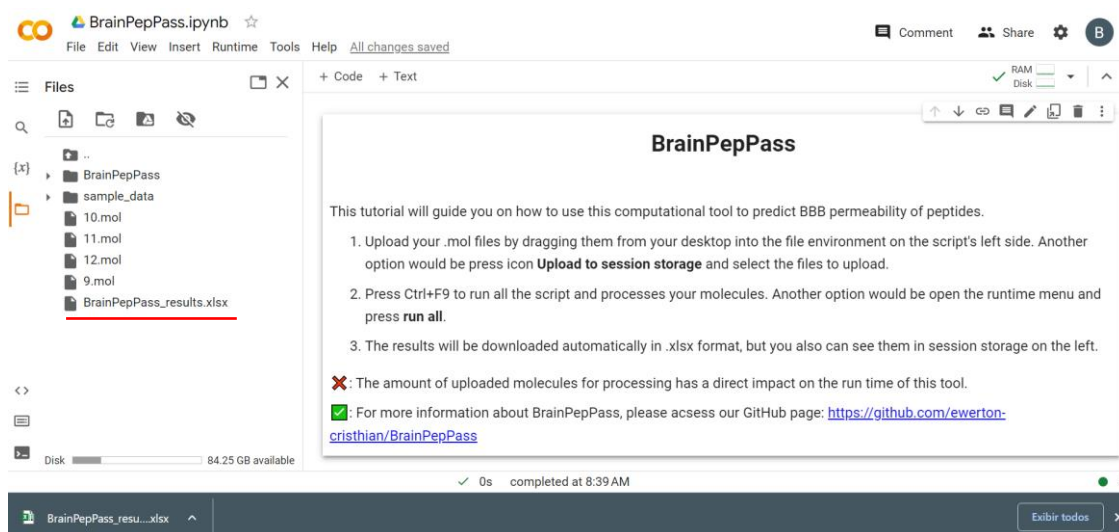


Figure 6: Download and availability of the results.